

**INPUT TO SAFETY EVALUATION REPORT  
ON DISPOSAL CRITICALITY ANALYSIS  
METHODOLOGY TOPICAL REPORT**

*Prepared for*

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## QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

**DATA:** There are no original data contained in this report.

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## 2 STAFF EVALUATION CRITERIA

To evaluate the U.S. Department of Energy (DOE) proposed approach in analyzing the potential for and consequences of criticality events at the proposed Yucca Mountain (YM) repository, a set of documents has been developed establishing the requirements that must be met to demonstrate compliance with the applicable regulations. The following sections provide a brief description of these pertinent documents. In addition, the regulatory requirements and guidance related to disposal criticality contained in each of these documents are presented.

### 2.1 Proposed Code of Federal Regulation Title 10, Part 63

The overall licensing criteria for the disposal of spent nuclear fuel and high-level radioactive waste in the proposed geologic repository at YM, Nevada, are included in the proposed 10 Code of Federal Regulations (CFR) Title 10, Part 63 (Nuclear Regulatory Commission, 1999a). This proposed regulation was published for public comment in the February 22, 1999, issue of the Federal Register. The public comments are being addressed by the Nuclear Regulatory Commission (NRC) at the present time. Furthermore, the U.S. Environmental Protection Agency (EPA) has issued the proposed 40 CFR Part 197 (U.S. Environmental Protection Agency, 1999) for public comment. The proposed 40 CFR Part 197 establishes the public health and safety standard for radioactive material stored or disposed in the potential repository at YM, Nevada. Under the Energy Policy Act of 1982, NRC regulations in the final 10 CFR Part 63 must be consistent with the final EPA Standard for YM. Depending on the final resolution of the public comments on both the proposed 10 CFR Part 63 and 40 CFR Part 197, some of the quantitative measures provided in the proposed 10 CFR Part 63 may change.

The proposed 10 CFR Part 63 specifies the overall performance objectives for the preclosure and postclosure phases of the repository. The DOE topical report (TR) however, only addresses postclosure criticality. The specification for overall performance of the repository with respect to postclosure is expected annual dose to the average member of the critical group. In keeping with the Commission philosophy of risk-informed, performance-based regulation, there are no specific design criteria for postclosure criticality control in the proposed 10 CFR Part 63. Criticality is a process that must be considered in the assessment to demonstrate that the system meets the overall system requirements in 10 CFR 63.113 as demonstrated with a performance assessment conducted in accordance with the requirements of 10 CFR 63.114, as quoted in the following paragraphs:

*63.113 (b) The engineered barrier system shall be designed so that, working in combination with natural barriers, the expected annual dose to the average member of the critical group shall not exceed 0.25 mSV (25 mrem) TEDE at any time during the first 10,000 years after permanent closure, as a result of radioactive materials released from the geologic repository.*

*63.114 Any performance assessment used to demonstrate compliance with §63.113 shall: . . . (d) Consider only events that have at least one chance in 10,000 of occurring over 10,000 years. (e) Provide the technical basis for either inclusion or exclusion of specific features, events, and processes of the geologic setting in the performance assessment. Specific features, events, and processes of the geologic setting must be evaluated in detail if the magnitude and time of the resulting expected annual dose would be significantly*

*changed by their omission. (f) Provide the technical basis of either inclusion or exclusion of degradation, deterioration, or alteration processes of engineered barriers in the performance assessment, including those processes that would adversely affect the performance of natural barriers. Degradation, deterioration, or alteration processes of engineered barriers must be evaluated in detail if the magnitude and time of the resulting expected annual dose would be significantly changed by their omission.*

The staff has used the foregoing requirements in evaluating the DOE proposed approach for addressing the postclosure criticality aspect of spent nuclear fuel and high-level waste (HLW) disposal in the YM. These requirements are translated into specific acceptance criteria (AC) and review methods (RMs) for disposal criticality control subsystems described in the various issue resolution status reports (IRSRs) (Nuclear Regulatory Commission, 1999b-d, 2000). Eventually all the AC and RMs for criticality control subsystems will be included in the YM Review Plan (YMRP). The IRSRs will contain only the status of the issue resolution.

**2.2 Draft Yucca Mountain Review Plan**

The draft YMRP is currently being developed at the NRC. This document will be used to review the DOE's future license application (LA) to ensure that the LA meets the requirements of 10 CFR Part 63. The YMRP will be used to assess the adequacy of both the preclosure and postclosure safety assessments performed for the repository system ensuring that the LA demonstrates the site will meet all the requirements of 10 CFR Part 63. Currently, the AC and RMs associated with the resolution of postclosure issues are located in the IRSRs, of the various key technical issues (KTIs). These AC and RMs will be removed from the IRSRs, however, and incorporated into the YMRP when Revision 1 of the YMRP is released (expected in September 2000).

Review of the postclosure performance assessment using the YMRP will be based on an integrated subissue (ISI) framework. The ISIs are the integrated features, events, and processes (FEPs) that could impact system performance. The effects of postclosure criticality will be addressed under the following ISIs in the YMRP: Degradation of Engineered Barriers, Quantity and Chemistry of Water Contacting Waste Packages and Waste Forms, Radionuclide Release Rates and Solubility Limits, Radionuclide Transport in the Unsaturated Zone, Radionuclide Transport in the Saturated Zone, and Mechanical Disruption of Engineered Barriers.

The potential for criticality during preclosure operations will be assessed in the preclosure section of the YMRP. The proposed methodology in the DOE TR, however, applies only to assessing the probability and consequences of a postclosure criticality event and does not apply to preclosure criticality. Therefore, preclosure criticality will not be discussed in this safety evaluation report (SER).

**2.3 Issue Resolution Status Reports**

The NRC strategic planning assumptions call for the early identification and resolution, at the staff level, of issues before the receipt of a potential LA to construct a geologic repository. The principal means for achieving this goal is through informal, preclicensing consultations with the DOE. These consultations, required by law, occur in an open manner that permits observation by the State of Nevada, Tribal Nations, affected units of local government, and interested members of the public. Obtaining input and

striving for consensus from the technical community and interested parties help the issue resolution process. The issue resolution approach reduces the number of, and better defines, issues that may be in dispute during the NRC licensing review.

Thus, consistent with the NRC regulations and a 1993 agreement with the DOE, staff-level issue resolution can be achieved during the prelicensing consultation period; however, such resolution at the staff level would not preclude the issue being raised and considered during licensing proceedings. Issue resolution at the staff level during prelicensing is achieved when the staff have no further questions or comments (i.e., open items) concerning the DOE approach to addressing an issue. There may be some cases where resolution at the staff level may be limited to documenting a common understanding regarding differences in the NRC and DOE technical positions. Pertinent, additional information could raise new questions or comments regarding a previously resolved issue.

An important step in the staff's approach is to provide DOE with feedback regarding issue resolution before the forthcoming Site Recommendation and LA. IRSRs are the primary mechanism that the NRC staff will use to provide DOE with feedback on KTI subissues. IRSRs focus on (i) AC for issue resolution and (ii) the status of resolution, including areas of agreement or when the staff has comments or questions. Open meetings and technical exchanges with DOE have provided, and will continue to provide, additional opportunities to discuss issue resolution, identify areas of agreement and disagreement, and develop plans to resolve such disagreements. An important goal of these prelicensing interactions is to exchange sufficient information to reach closure on the open items by the time the LA is submitted by the DOE.

**2.3.1 Total System Performance Assessment and Integration**

Postclosure criticality is planned to be treated as a disruptive scenario by the DOE in the performance assessment conducted for YM. The treatment of criticality within the total system performance assessment (TSPA) is considered acceptable if the following AC from the total system performance assessment and integration (TSPAI) IRSR (Nuclear Regulatory Commission, 2000) are met:

- 1. *“DOE has identified a comprehensive list (i) of processes and events that are present or might occur in the YM region and (ii) that includes those processes and events that have the potential to influence repository performance.*
- 2. *“DOE has provided adequate documentation identifying how its initial list of processes and events have been grouped into categories.*
- 3. *“Categorization of processes and events is compatible with the use of categories during the screening of processes and events.*
- 4. *“The probability assigned to each category of processes and events is consistent with site information, well documented, and adequately considers uncertainty.*
- 5. *“Processes and events screened from the PA on the basis of their probability of occurrence, have been demonstrated to have a probability of less than one chance in 10,000 of occurring over 10,000 years.*

- 6. *“DOE has demonstrated that categories of processes and events omitted from the PA based on low consequence would not significantly change the calculated expected annual dose.*
- 7. *“DOE has provided adequate documentation identifying: (i) whether processes and events have been addressed through consequence model abstraction or scenario analysis and (ii) how the remaining categories of processes and events have been combined into scenario classes.*
- 8. *“The set of scenario classes identified by DOE is mutually exclusive and complete.*
- 9. *“Scenario classes that are not credible for the YM repository because of waste characteristics, repository design, or site characteristics—individually or in combination—have been identified and sufficient justification has been provided for DOE’s conclusions.*
- 10. *“The probability assigned to each scenario class is consistent with site information, well documented, and appropriately considers uncertainty.*
- 11. *“DOE has demonstrated that for scenario classes screened from the PA on the basis of their probability of occurrence: (i) the probability used for screening the scenario class is defined from combinations of initiating processes and events and (ii) DOE has demonstrated that they have a probability of less than one chance in 10,000 of occurring over 10,000 years.*
- 12. *“Scenario classes omitted from the PA on the basis of low consequence have been demonstrated to not significantly change the calculated expected annual dose.”*

If criticality is included in the TSPA analyses, the model abstraction for criticality should meet the five AC in the YMRP on model abstraction:

- 13. *“Sufficient data (e.g., field, laboratory, and natural analog data) are available to adequately define relevant parameters and conceptual models necessary for developing the abstraction in the TSPA. Where adequate data do not exist, other information sources such as expert elicitation have been appropriately incorporated into the TSPA.*
- 14. *“Parameter values, assumed ranges, probability distributions, and bounding assumptions used in the TSPA abstraction are technically defensible and reasonably account for uncertainties and variabilities.*
- 15. *“Alternative modeling approaches consistent with available data and current scientific understanding are investigated and results and limitations are appropriately considered in the abstractions.*

16. *“Models implemented in the TSPA provide results consistent with output of detailed process-level models or empirical observations (e.g., laboratory testing, field measurements, or natural analogs).”*
17. *“TSPA adequately incorporates important design features, physical phenomena and couplings, and uses consistent and appropriate assumptions throughout the abstraction process.”*

Additionally, all data and computer codes used in the criticality abstraction should meet the following acceptance criterion related to quality assurance (QA):

18. *“The collection, documentation, and development of data, models, and computer codes have been performed under acceptable quality assurance (QA) procedures, or if the data, models, or computer codes were not subject to an acceptable QA procedure, they have been appropriately qualified.”*

Finally, formal expert elicitations can be used to support data synthesis and model development for DOE’s criticality abstraction, provided that the elicitations meet the following acceptance criterion or the DOE can demonstrate in other ways that the conduct of the elicitations provides an adequate level of confidence in the results:

19. *“Formal expert elicitations used to support data synthesis and model development for DOE’s TSPA have been conducted and documented under acceptable procedures.”*

### **2.3.2 Container Life and Source Term**

The container life and source term (CLST) IRSR (Nuclear Regulatory Commission, 1999b) contains AC related to how the conditions inside the waste package (WP) could influence the occurrence of criticality and how in-package criticality could affect WP and engineered barrier subsystem performance. The evaluation of the probability and consequences of in-package criticality on WP and engineered barrier subsystem performance will be acceptable if the following AC are met:

1. *“Mathematical model limitations and uncertainties in modeling were defined and documented.”*
2. *“Primary and alternative modeling approaches consistent with available data and current scientific understanding were investigated and their results and limitations considered in evaluating the subissue.”*
3. *“DOE has used sound technical bases for selecting the design criteria for components to mitigate any potential effects of in-package criticality on the repository performance. These design criteria may include development of subcritical limit, probability and consequence of criticality, and any other design criteria considered to be necessary by DOE.”*

4. *“DOE has identified all the features, events, and processes that may increase the reactivity of the system inside the WP.*
5. *“DOE has identified the configuration classes and configurations that have potential for nuclear criticality. If models are used to develop the configuration, approach and accuracy in modeling verification and validation will be evaluated.*
6. *“DOE has developed a technically defensible, transparent, and traceable method in assigning probability values to each of the scenario classes, scenarios, configuration classes, and configurations.*
7. *“DOE has developed appropriate computer models, input parameters, and determined quantitative values for calculating the effective neutron multiplication factor ( $k_{eff}$ ), including appropriate biases and uncertainties in the model.*
8. *“DOE has developed appropriate computer models, evaluated input parameters, and determined quantitative values for calculating the radionuclide inventory, heat, kinetic energy, and other parameters that would change as a result of  $k_{eff}$  exceeding the subcritical limit developed under Criterion (3).*
9. *“DOE has determined the risk contribution from the in-package criticality to the total repository system performance appropriately.”*

### **2.3.3 Evolution of the Near-Field Environment**

The evolution of the near-field (NF) environment IRSR (Nuclear Regulatory Commission, 1999c) contains AC related to how the NF conditions could influence the occurrence of criticality and how nuclear criticality outside of the WP affects the NF environment. The evaluation of the probability and consequences of criticality in the NF environment will be acceptable if the following AC are met:

1. *“Sensitivity and uncertainty analyses (including consideration of alternative conceptual models) were completed to determine whether criticality will impact repository performance, and whether additional new data are needed to better define ranges of input parameters.*
2. *“Available data relevant to both temporal and spatial variations in conditions affecting coupled (THC) effects on the potential for nuclear criticality in the near-field environment were considered.*
3. *“DOE’s evaluation of coupled THC processes properly considered site characteristics in establishing initial and boundary conditions for conceptual models and simulations of coupled processes that may affect nuclear criticality in the near-field environment.*
4. *“Sufficient data were collected on the characteristics of the natural system and engineered materials, such as the type, quantity, and reactivity of material, in*

*establishing initial and boundary conditions for conceptual models and simulations of THC coupled processes that may affect nuclear criticality in the near-field environment.*

5. *“Reasonable or conservative ranges of parameters or functional relations were used to determine effects of coupled THC processes on potential nuclear criticality in the near-field environment. Parameter values, assumed ranges, probability distribution, and bounding assumptions are technically defensible and reasonably account for uncertainties.*
6. *“Uncertainty in data due to both temporal and spatial variations in conditions affecting coupled THC effects on potential nuclear criticality was considered.*
7. *“DOE’s evaluation of coupled THC processes properly considered the uncertainties in the characteristics of the natural system and engineered materials, such as the type, quantity, and reactivity of material, in establishing initial and boundary conditions for conceptual models and simulations of THC coupled processes that affect potential nuclear criticality.*
8. *“The initial conditions, boundary conditions, and computational domain used in sensitivity analyses involving coupled THC effects on potential nuclear criticality in the near-field environment were consistent with available data.*
9. *“Alternative modeling approaches consistent with available data and current scientific understanding were investigated, and their results and limitations were appropriately considered.*
10. *“DOE provided a reasonable description of the mathematical models included in its analyses of coupled THC effects on potential nuclear criticality. The description should include a discussion of alternative modeling approaches not considered in its final analyses and the limitations and uncertainties of the chosen model.*
11. *“The mathematical models for coupled THC effects on potential nuclear criticality are consistent with conceptual models based on inferences about the near-field environment, field data and natural alteration observed at the site, and expected engineered materials.*
12. *“DOE appropriately adopted accepted, and well-documented, procedures to construct and test the numerical models used to simulate coupled THC effects on potential nuclear criticality.*
13. *“Abstracted models for coupled THC effects on potential nuclear criticality were based on the same assumptions and approximations shown to be appropriate for closely analogous natural or experimental systems. Abstracted model results were verified through comparison to outputs of detailed process models and empirical observations. Abstracted model results are compared with different mathematical models to judge robustness of results.*

- 14. *“DOE has considered all the relevant features, events, and processes. The abstracted models adequately incorporated important design features, including criticality safety features; physical phenomena and couplings, including neutron absorbers; and used consistent and appropriate assumptions throughout.*
- 15. *“Important mass transfer and mass transport processes and mechanisms considered for formation of both a critical mass and configuration are plausible for the YM near-field environment.*
- 16. *“Models reasonably accounted for known temporal and spatial variations in conditions affecting coupled THC effects on potential nuclear criticality.*
- 17. *“Criticality in the near field, and not all THC couplings, may be determined to be important to performance, and DOE may adopt assumptions to simplify PA analyses. If potentially important couplings and criticality in the near field are neglected, DOE should provide a technical basis for doing so. The technical basis could include activities, such as independent modeling, laboratory or field data, or sensitivity studies.*
- 18. *“Where simplifications for modeling coupled THC effects on potential nuclear criticality were used for PA analyses instead of detailed process models, the bases used for modeling assumptions and approximations were documented and justified.*
- 19. *“Data and models were collected, developed, and documented under acceptable QA procedures.*
- 20. *“Deficiency reports concerning data quality on issues related to coupled THC effects on the potential for nuclear criticality were closed.*
- 21. *“If used, expert elicitations were conducted and documented in accordance with the guidance in NUREG-1563 (Nuclear Regulatory Commission, 1996) or other acceptable approaches.”*

**2.3.4 Radionuclide Transport**

The radionuclide transport IRSR (Nuclear Regulatory Commission, 1999d) contains AC related to how the far-field (FF) conditions could influence the occurrence of criticality and how nuclear criticality outside of the WP could affect the FF environment. The evaluation of the impacts of criticality outside of the repository drifts will be acceptable if the following AC are met:

- 1. *“The DOE has properly considered site characteristics. Analyses are consistent with hydrology, geology, and geochemistry observed during site characterization in the YM system. These data should include realistic rock chemistry, rock porosity, and water chemistry.*

2. *"The DOE has properly considered repository, WP, and waste form design in establishing initial and boundary conditions. Parameters and conceptual models for nuclear criticality as a result of radionuclide transport to the far field are consistent with the current repository and waste form design for the YM repository.*
3. *"The DOE has, where process modeling studies have been used, documented preferred and alternative conceptual models that are supported by available data, analyses, and interpretations, and are both internally consistent and consistent with other applications of radionuclide transport models. Adequate basis is provided for excluding potentially adverse phenomena.*
4. *"The DOE has demonstrated that mathematical models are consistent with conceptual models based on field data and field observations at the site. Mathematical model limitations and uncertainties in modeling nuclear criticality due to radionuclide transport are defined and documented. Models are validated by comparison with data from field, laboratory, and natural analog studies.*
5. *"The DOE has performed sensitivity and uncertainty analyses (including consideration of alternative conceptual models) to determine if models are overly optimistic and to help determine whether additional new data are needed to better define ranges of input parameters.*
6. *"The DOE has collected, developed, and documented data and models under acceptable QA procedures (e.g., Altman, et al., 1988). Where necessary, data qualification plans are acceptable, and data uncertainties have been identified and documented. Data uncertainties are propagated correctly or are conservative with regard to repository performance. It should be verified that there are no deficiency reports, concerning data quality in relation to nuclear criticality as a result of radionuclide transport that have not been closed.*
7. *"The DOE has, where data are not reasonably or practicably obtained, used expert judgement appropriately and adequately documented expert elicitation procedures. If used, expert elicitations were conducted and documented in accordance with the guidance in NUREG-1563 (Nuclear Regulatory Commission, 1996) or other acceptable approaches.*
8. *"The DOE has used appropriate models for estimating worst-case radionuclide inventory increases due to far field criticality events.*
9. *"The DOE has evaluated the effects of criticality event thermal output in the far field, with consideration of coupled THC processes that may affect hydrologic conditions.*
10. *"The DOE has appropriately applied criticality effects in TSPA models assessing performance consequences. The DOE has used model parameter estimates that ensure that the analysis is not overly optimistic. Such parameters include*

*radionuclide inventory increase and conservative estimates of the number and timing of far field criticality events. Performance consequences are evaluated in the context of uncertainties and sensitivities established for TSPA.*

11. *“DOE has demonstrated that important mass transfer and mass transport processes and mechanisms affecting formation of both a critical mass and configuration are plausible for the YM environment.*
12. *“DOE has demonstrated that the method for establishing scenarios has a reasonable assurance of not excluding any credible scenarios. Preferred and alternative conceptual models have been documented and are supported by available data, analyses, and interpretations, and are internally consistent.*
13. *“DOE has provided conceptual models and quantitative values for effective neutron multiplication factors to demonstrate whether a given configuration of fissile radionuclides will remain subcritical ( $k_{eff} < 1$ ) or become critical ( $k_{eff} \geq 1$ ).*
14. *“DOE has provided reasonable assurance that exclusion of configurations based on an estimated  $k_{eff} < 1$  has effectively demonstrated that those configurations are not credible. For example, DOE may establish a safety factor by establishing a lower value of  $k_{eff}$  as a cutoff for configurations considered not credible.*
15. *“DOE has established an appropriate probability screening level for estimating the credibility of criticality for a given configuration.”*

## **2.4 Applicable Regulatory Guides and Standards**

There are no formal regulatory guidance documents or industry standards specific to criticality in a permanent HLW repository. Existing guides may be followed in formulating and assessing disposal criticality analyses. In conducting its review of the TR, the NRC has referred to Regulatory Guide 3.71, Nuclear Criticality Safety Standards for Fuels and Material Facilities (Nuclear Regulatory Commission, 1998). This is an appropriate guide to follow because it concerns criticality analyses supporting safety in handling, storage, and transportation outside reactors. Regulatory Guide 3.71 replaces several earlier guides (3.1, 3.4, 3.43, 3.45, 3.47, 3.57, 3.58, 3.68, 3.70, and 8.12) and recommends that licensees follow procedures outlined in several American National Standards Institute (ANSI)/American Nuclear Society (ANS)-8 nuclear criticality safety standards, supplemented by a detailed, operation-specific criticality analysis.

In developing the criticality methodology, the DOE has applied guidance from NRC regulatory guides as well as from industry standards. From NUREG/CR-2300 (Nuclear Regulatory Commission, 1983), the DOE has borrowed the approach to probabilistic risk assessment (PRA) for nuclear power plants and modified it for postclosure disposal criticality analysis. The three steps of PRA—scenario analysis, failure and release, and environmental transport and exposure—may be mapped in general terms to the three key steps of the disposal methodology: scenario analysis, source term, and input of source term into TSPA. Two other NUREGs—NUREG/CR-6361 (Lichtenwalter et al., 1997) and NUREG/CR-5661 (Nuclear Regulatory Commission, 1997)—have been used for criticality model benchmarking and

establishing criticality limits, respectively. These two NUREGs cite a subset of the ANSI/ANS standards discussed by the TR: ANSI/ANS-8.1, 8.15, 8.17, and 8.10, which are concerned with criticality control of fissionable materials outside of reactors (e.g., during transport or in nonreactor facilities). Application of the standards to disposal criticality is not direct, but is established by analogy. Finally, the TR cites two NRC Regulatory Guides: 3.4 (Nuclear Regulatory Commission, 1986a) and 3.58 (Nuclear Regulatory Commission, 1986b), which are again concerned with criticality analyses supporting safety in handling, storage, and transportation. These regulatory guides endorse ANSI/ANS-8.1 and 8.17. The TR states that the disposal criticality methodology is consistent with these guides with the exception of the TR approach to burnup confirmation. The DOE states it does not plan to necessarily measure reactivity on each fuel bundle and may rely on burnup inferences (see last paragraph of this section).

In the absence of formal regulatory guidance documents or industry standards applicable to permanent HLW disposal, the DOE supports application of these materials by analogy. For example, a level 1 PRA "consists of an analysis of plant design and operation focused on the accident sequences that could lead to core melt, their basic causes, and their frequencies" (Nuclear Regulatory Commission, 1983). This analysis is deemed analogous to the DOE method for constructing scenarios and configuration classes that define the possible ways in which criticality may occur in the repository. The DOE cites cases in which strict adherence to the standards is inappropriate. For example, in applying ANSI/ANS-8.1, single-parameter limits and the double-contingency criterion are deemed inadequate for a complex repository system. The DOE does not necessarily intend to strictly follow regulatory guidance and industry standards because they are not specific to a repository system. Justification for model approaches, parameters, limits, and validations are described elsewhere in the TR, with the cited guidance and standards providing starting points for development of the DOE approach.

Recently, NRC Regulatory Guides 3.4 and 3.58 have been subsumed into Regulatory Guide 3.71, with no changes in licensing commitments or requirements. In its response to the NRC request for additional information (RAI) 2-1, the DOE stated that it will revise section 2.3.3 of the TR to refer to the newer 3.71 in place of other regulatory guides.

The NRC approves of the DOE approach to the use of regulatory guides and standards in the criticality analysis, with one condition. NRC Regulatory Guide 3.71 (Nuclear Regulatory Commission, 1998) states in section C that safety criteria for preventing nuclear criticality described in ANSI/ANS-8.17-1997 are acceptable as guidance, with one exception. This exception is that "credit for fuel burnup may be taken only when the amount of burnup is confirmed by physical measurements that are appropriate for each type of fuel assembly in the environment in which it is to be stored." In contrast, the DOE states in section 2.3.3 of the TR that it may not perform reactivity or flux measurements on all spent fuel bundles, but rather may depend in some cases on inferred burnups. This variance from Regulatory Guide 3.71 is not acceptable, and this issue is considered an open item.

### **3.3 Criticality Scenarios**

#### **3.3.1 Internal Criticality Scenarios (Sections 3.1, 3.1.1)**

The DOE has proposed a master scenario list that consists of a standard set of degradation scenarios that must be considered as part of the criticality analysis of any waste form (WF) disposed in the repository. Section 3.1 of the TR provides a description of the internal scenarios that will be evaluated for criticality.

In its responses to the RAI, DOE has requested approval of the master scenario list as stated by the DOE in the following paragraph:

*DOE requests acceptance that the list of standard scenarios outlined in Figures 3-1 and 3-2, as supplemented by the new Sections 3.1.3 and 3.1.4 to be added to the Topical Report as discussed in the response to RAI 3-1, comprehensively identifies the generic degradation scenarios incorporating those features, events, and processes associated with the proposed repository at Yucca Mountain that may significantly affect the potential for, and consequences of, criticality.*

The development of degradation scenarios is based on a combination of FEPs within the YM repository that result in degraded configurations to be evaluated for criticality. Groups of similar degraded configurations are combined into configuration classes to reduce the calculational burden while ensuring that a comprehensive set of configurations is considered. These configuration classes consist of configurations with similar material compositions and geometries that differ due to parameters, such as uranium enrichment and burnup or water infiltration rate, which vary over a given range.

The internal scenarios are combinations of FEPs that may result in critical configurations inside the WP and are determined based on several discriminators. The top-level discriminator is whether the location of the initial WP penetration is at the top or bottom of package, which determines whether water can accumulate inside the package. The second level discriminator is the rate of degradation of the WP internal structures as compared to the degradation of the WF. Lower-level discriminators include items such as the transport characteristics of the fissile materials (FMs) and structural materials. These scenarios can result in the following configuration classes, which the DOE has identified as having the potential to support a criticality event and, therefore, requiring analysis for all WFs:

- The WP internals are degraded, but the WF remains relatively intact. Criticality is possible if water fills the lower portion of the package, neutron absorber is flushed from the WP, and little fissionable material is removed from the package.
- Both the WP internal structure and WF are degraded and resting on the bottom of the WP. There is a criticality potential if water fills the lower portion of the package, absorbing material is flushed out of the package, and most of the fissionable material remains within the WP.
- The WP internals remain relatively intact, but the WF is degraded. A criticality event could be possible if water fills the lower portion of the package and the degradation of the WF causes physical separation between the fissionable material and the neutron absorber.
- The WF accumulates at the bottom of the WP along with water trapped in clay or with hydrated corrosion products without any standing water in the package.
- The fissionable material is trapped along with water in clay filling the WP and distributed throughout the WP volume.

- The WF degrades in place with the WP internals intact. No additional separation is created between the fissionable materials and the neutron absorbers in the WP internal components, but the degraded WF is more reactive than the intact WF for some fuel types.

The DOE, per response to RAI 3-1, has addressed how disruptive events such as seismicity and volcanism will be evaluated in the master scenario list. Seismic events will be addressed by identifying representative seismic predecessor configurations that could be transformed to one of the six previously identified critical configurations by a seismic event. These critical configurations are distinguished by the level of degradation of the basket and the WF. The predecessor configurations will have significantly higher gravitational potential energy than the critical configurations such that a seismic event could rearrange the materials to form critical configurations. The seismic event could increase the reactivity of the system by shifting fuel assemblies such that more assemblies fall below the water level in the WP, causing individual fuel pins to collect in a more compact configuration, or moving poison or moderator-excluding materials such as the basket structure of corrosion products away from the fuel and replacing them with water. A critical configuration created by a seismic event would likely lead to a transient criticality due to the relatively short period of time that reactivity is inserted. The probability of the occurrence of a transient criticality initiated in this manner would be determined by considering both the probability of occurrence of the predecessor configuration and the probability of a seismic event of sufficient magnitude occurring to take such configurations to criticality. The probability and consequences of the transient criticality will be used to determine a transient criticality risk due to seismicity.

The NRC staff reviewed the master scenario list against the AC in the IRSRs to determine whether all FEPs that have the potential to increase the reactivity of the system inside the WP can be evaluated in the identified scenarios (CLST AC #4) or can be eliminated on the basis of low probability (TSPAI AC #11) or low consequence (TSPAI AC #12). Additionally, staff review determined whether a comprehensive list of processes and events have been identified (TSPAI AC #1) and whether adequate documentation was provided identifying how the initial list of processes and events were grouped into categories (TSPAI AC #2). Staff review was supplemented by examination of a preliminary DOE FEPs database (U.S. Department of Energy, 1999) to ensure that the FEPs identified as important to the criticality evaluation inside the WP in the FEPs database can be accounted for with the master scenario list.

The NRC staff found that grouping sets of similar configurations into configuration classes is a reasonable way to reduce the calculational burden but still provide reasonable assurance that the probability of criticality will not be significantly underestimated. The NRC staff found that the master scenario list and the additional analyses conducted for seismic events as stated in the response to RAI 3-1 will adequately identify scenarios that may significantly impact the potential for or consequences of a criticality event within the WP based on the FEPs associated with the YM repository. The NRC staff found that all FEPs important to the criticality evaluation inside the WP can be incorporated in the proposed methodology if the additional steps accounting for seismic events are performed.

### 3.3.2 External Criticality Scenarios (Sections 3.1, 3.1.2)

A component of the DOE request discussed in section 3.3.1 is acceptance of the list of external scenarios in figure 3-2 of the TR. External scenarios are combinations of FEPs that may result in critical configurations outside the WP. These scenarios, classified as NF or FF depending on their location

relative to the drift walls, are preceded by one or more internal scenarios (section 3.3.1 of this SER) that result in release of FM from the WP. (There is one exception, scenario NF-5.) Simplified descriptions of the DOE scenarios are as follows; note that the invert is assumed to contain concrete, crushed tuff, or both.

- NF-1: solute transport of FM from the WP and accumulation in the invert
- NF-2: slurry transport of FM from the WP and accumulation on the invert
- NF-3: colloidal transport of FM from the WP and accumulation in the invert
- NF-4: water ponds in drift, WP and WF degrade, and FM accumulates in clays at the bottom of the drift
- NF-5: water ponds in drift, WP degrades, and intact WF sits in pond

- FF-1: solute transport of FM from the drift and chemical accumulation in the unsaturated zone
- FF-2: colloidal transport of FM from the drift and accumulation in the unsaturated zone
- FF-3: solute transport of FM from the drift and chemical accumulation in the saturated zone

All scenarios require—in addition to release and transport of FM—a degree of separation of FM from neutron absorbers, and mechanisms for this process are therefore included. Each scenario encompasses one or more configuration classes, which further specify the processes and setting that define the potentially critical configuration. For example, scenario NF-3 includes three configuration classes—NF-3a, NF-3b, and NF-3c—that specify whether colloids accumulate in WP corrosion products, invert fractures, or degraded concrete, respectively.

The DOE constructed and validated this list of external scenarios and configuration classes as part of the Total System Performance Assessment—Viability Assessment (TSPA-VA) abstraction effort, and were thus informed by the comprehensive, site-specific TSPA scenario analysis (U.S. Department of Energy, 1998). The list was produced at a DOE workshop and reviewed by a group of experts. The expert review constitutes the DOE validation of the process of identifying scenarios.

The DOE provided additional, clarifying information in its responses<sup>1</sup> to NRC RAI items 3-2, 3-4, 3-5, 3-6, 3-7, and 3-8 that resolved NRC questions on external scenarios.

- RAI 3-2. In response to the NRC comment that the DOE should include external scenarios with potentially positive neutronic feedback characteristics, the DOE stated that such configurations (a more appropriate term than scenarios) are explicitly included in the TR discussion of criticality consequence modeling (section 4.4.1.2).
- RAI 3-4, 3-5, 3-6, 3-7, and 3.8. These items dealt with either (i) inappropriate wording in the TR that gave the erroneous impression that certain processes or mechanisms were excluded when configuration classes were defined or (ii) editorial ambiguities. For example, RAI 3-5 pointed out that the TR appeared only to be considering reduction as a mechanism for FM precipitation. The DOE will change the TR to reflect the fact that reduction is merely an example of the possible mechanisms.

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<sup>1</sup>Brocoum, S. *U.S. Department of Energy (DOE) Response to U.S. Nuclear Regulatory Commission (NRC) Request for Additional Information on the DOE Topical Report on Disposal Criticality Analysis Methodology*. Letter (November 19) to C.W. Reamer, Nuclear Regulatory Commission. Las Vegas, NV: U.S. Department of Energy. 1999.

The occurrence of igneous activity in the repository would lead to a configuration significantly different from those identified in the master scenario list, so DOE will provide a completely separate analysis to determine the criticality potential from a volcanic event. This analysis, as described in response to RAI 3-1 will consist of a probabilistic methodology to determine the probability of a criticality event following an igneous intrusion. The analysis will consist of the following four steps: (i) evaluating the probability of the WP breaching during a volcanic event, (ii) modeling the transport of fissionable material following breach of the WP, (iii) determining the accumulation of fissionable material from the magma flow, and (iv) determining the potential for criticality of any accumulations identified using silica, water moderation, or both, as appropriate.

If the probability of criticality resulting from igneous activity exceeds the TSPA screening level of  $10^{-8}/\text{yr}$  for the entire repository, the consequences of these criticality events will have to be determined to evaluate the risk associated with such an event.

Staff assessed the comprehensiveness of the DOE scenario list with reference to NRC and DOE documents concerned with FEPs external to the WP. In particular, NRC IRSRs on the evolution of the near-field environment (ENFE) (Nuclear Regulatory Commission, 1999a) and radionuclide transport (RT) (Nuclear Regulatory Commission, 1999b) KTIs provided extensive discussions on the range of FEPs that may affect the fate and transport of contaminants, including FMs and neutron absorbers, in the NF and FF. This assessment applied AC from these two IRSRs, as well as from the TSPAI IRSR (Nuclear Regulatory Commission, 2000), listed in section 2.3 of this SER. From section 2.3.1 (TSPAI), relevant criteria are numbers 1, 2, 3, 7, and 8 concerned with the establishment and categorization of a scenario list. From section 2.3.3 (ENFE), criteria relevant to scenarios are 14 and 15. From section 2.3.4 (RT), criteria 11 and 12 were applied. In general terms, these criteria are concerned with the construction of scenario lists that are comprehensive, consistent with site and design characteristics, and categorized in a manner facilitating scenario screening. Staff review was supplemented by examination of a preliminary DOE FEPs database (U.S. Department of Energy, 1999a). Specifically, the database was checked for (i) inclusion of all external scenarios delineated in the TR and (ii) inclusion of any external scenarios not in the TR.

NRC staff found that—contingent on the TR revisions promised in the DOE RAI responses and on addressing an additional scenario described in the next paragraph—the external master scenario list, as depicted in figure 3-2 of the TR and described in section 3.1 of the TR, comprehensively identifies generic, site-specific scenarios that may impact significantly the potential for, and consequences of, a criticality event external to the WP at YM. The scenarios cover the range of reasonably conceivable physical and chemical processes that could affect the external disposition of FM and neutron absorbers. The integration of the criticality scenario analysis with the TSPA scenario analysis lends confidence to the criticality effort because the DOE increasingly is making scenario analysis a transparent process that the NRC can readily evaluate. The criticality scenario list should be flexible enough to respond to any future changes in the TSPA scenario analysis. For example, design changes affecting the composition and dimensions of the invert will affect the viability and completeness of the scenarios involving invert accumulation of FM. NRC staff found the framework that the DOE presented in the response to RAI 3-1 to analyze the probability of igneous-activity-induced criticality is acceptable. The response to the RAI, however, does not present a sufficient level of detail about how each of the four steps in the analysis will be conducted to make a finding whether the analysis will be considered appropriate by NRC staff.

One potential exception to the comprehensiveness of the TR scenario list was identified in the DOE FEPs database (U.S. Department of Energy, 1999a). Database entry 2.2.14.07.00 concerns FM precipitation due to dryout in a perched water basin, and is described as an "alteration" of configuration class FF-1a. NRC acceptance of the master scenario list is contingent on incorporation of this process into the scenario list, possibly by extending the definition of FF-1a.

### 3.4 Criticality Configurations

#### 3.4.1 Internal Configurations (Section 3.2, 4.2.1, 4.2.2)

The determination of internal configurations is based on the parameter ranges of the variables that describe the potentially critical internal configurations. In its responses to the RAI, DOE has requested an approval of the methodology for determining internal configurations as stated by the DOE in the following:

*DOE requests acceptance of the method for generating a comprehensive set of potential postclosure configurations as discussed in Sections 3.2 and 3.3 of the Topical Report. The principal components of this method are given in the following list.*

- *Degradation methodology: Ability of the methodology to calculate the loss of fissionable elements and neutron absorbers and calculate the composition of degradation products precipitating in the waste package. For this purpose we are requesting acceptance of the use of a steady-state geochemistry code. Improvements are still being incorporated into this methodology. The example discussed in the Topical Report (EQ3/6 in pseudo-flow-through mode, discussed in Section 4.2.2), has been replaced by the solid-centered-flow-through EQ3/6 code discussed in the response to RAI 4-32, which includes proposed modifications to Section 4.2.2. Use of this code is planned to be demonstrated and justified to support licensing.*
- *Configuration generator: (1) Use of time-dependent first-order differential equations, solved by numerical integration, to track the concentration, or amount of fissionable or neutron absorber material (Section 4.3.3); (2) Development of coefficients or terms of these equations by abstraction from steady-state geochemistry code calculations (Section 4.3.4); and (3) Random variation of terms or coefficients in these equations as part of a Monte Carlo calculation to reflect the uncertainty in the rates and location of natural processes (Section 4.3.4). In implementing #2, the appropriate balance between the use of EQ3/6 and the Configuration Generator Code will be demonstrated for each major waste form category as part of the License Application process. Examples of the use of #3 are given in Appendix C of the Topical Report, Sections 3.3 and 4.1, in response to RAI 4-38, and in CRWMS M&O, Probability of Criticality for MOX SNF, CAL-EBS-NU-000007.*
- *DOE requests acceptance of the validation process for the degradation analysis methodology that uses the solid-centered-flow-through mode (an*

*improvement on the pseudo-flow-through mode described in Section 4.2.2 of the Topical Report, as discussed in the response to RAI 4-32). DOE also requests acceptance for the validation process for accumulation methodology that uses a geochemistry-transport code or a geochemistry code used in a mode that simulates transport. This validation is expected to be provided by comparison between codes, comparison with experimental data, and comparison with natural analogs. These comparison cases are summarized in Tables 4-2 and 4-3 of the Topical Report. We do not seek acceptance of the bounding cases, which has been identified for the current range of environmental parameters and may be modified for the environmental parameters applicable to the Yucca Mountain repository that will support licensing.*

#### **3.4.1.1 Internal Configuration Methodology**

The proposed methodology to determine internal configurations is to use the appropriate range of configuration parameters to further specify the identified configuration classes for each combination of WF and WP. This methodology will be accomplished by performing a geochemical analysis for each configuration class to identify the chemical composition of the corrosion products remaining in the WP and by determining the physical properties of the remaining corrosion products. This end result will be specific and detailed range of configurations that must be considered in the parametric criticality evaluation of each configuration class.

The geochemical processes will be used to track the location of important fissionable, neutron moderating, and neutron absorbing materials and will be specified using the following steps:

1. Identify specific corrosion rates for all internal components, the range of drip rates of water onto a WP under a dripping fracture, and the range of dripping water chemistry parameters.
2. Estimate the location of potentially reacting materials to determine if a reaction is possible.
3. Perform probabilistic flow-through mode geochemical calculations for the representative parameter range for each configuration class.
4. Determine concentrations of fissionable materials and neutron absorbers in solution and in solids and insoluble corrosion products within the package.
5. Determine whether clay has formed from chemical alteration of glass WFs or from the silica and alumina in the water and the amounts of undegraded material and solid degradation products present.
6. Determine the range of hydration of degradation products possible if the package is not flooded.
7. Quantify the amounts of undegraded material and solid degradation products present for each configuration class.

8. Evaluate the potential for adsorption of soluble fissionable material or neutron absorbing material on corrosion products.

At appropriate intervals in the progress of the geochemical process, physical processes will be evaluated. These physical processes include possible locations for solids, the density and physical stability of corrosion products, the thermal and structural behaviors of the internal structures and the WF, and the effects of external events on the internal components, WF, or the location of the corrosion products.

The DOE, per response to RAI 1-4, has indicated they will evaluate the probability of occurrence of all configurations identified as potentially autocatalytic in published articles. This evaluation will provide additional confidence that all realistic potentially high-consequence criticality events have been considered.

The NRC staff reviewed the methodology that the DOE will use to identify critical configurations against the acceptance criteria in the IRSRs to ensure that the proposed methodology will identify the configuration classes and configurations that have potential for nuclear criticality (CLST AC #5). The methodology uses models to develop the configurations of interest, but acceptance of these computer codes is beyond the scope of the review of the topical report. Modeling verification and validation of these computer codes will be evaluated when DOE submits the appropriate validation reports.

The NRC staff found that, provided the DOE evaluates the probability of occurrence of all configurations identified as potentially autocatalytic in published articles as stated in the response to RAI 1-4, the proposed methodology is sufficient to provide reasonable assurance that the analysis has been performed on a comprehensive set of internal configurations and that no configuration that could increase substantially the calculation of the probability or consequence of a criticality event has been omitted from the analysis.

#### **3.4.1.2 Internal Configuration Modeling Approach**

The determination of internal criticality configurations depends on the degradation rate of WP barrier materials, internal components, and WFs determined from the quantity of water contacting the material and the chemistry of the dripping water.

Per response to RAI 4-25, individual corrosion models are developed based on data from the DOE material testing program for each of the materials that make up the WP and WF. WP degradation models will be the models used in the TSPA that output a distribution of breach times at various locations on the WP for a given set of environmental conditions. The degradation rates used in the criticality evaluation also will be consistent with the WF corrosion models used for TSPA.

The geochemistry within the WP will be calculated using a commercial software code such as EQ3/6 (Wolery, 1992). The software will be qualified under an appropriate QA program. A series of runs of the geochemistry code will be used to simulate water dripping into and leaking out of a WP. In response to RAI 4-32, the DOE stated that a modification to the EQ6 (Wolery and Daveler, 1992) portion of the code called the solid-centered-flow-through code, will be used to model water inflow and outflow and track the timestep adjustment.

The configuration generator code will be used to track the concentrations of neutronically significant isotopes and chemical species that can affect the solubility of the neutronically significant elements. This code uses time-dependent, first-order differential equations to represent the chemical transformations of elements or compounds that have coefficients determined by fitting data from detailed calculations of a geochemistry code such as EQ3/6 (Wolery, 1992). The code will provide bookkeeping for the transport between sites of the application of a detailed geochemistry code and, in some situations, provide more rapid calculation where the detailed geochemistry code results can be used to develop heuristic models for the most significant ions for a few solution parameters.

At each time step, the configuration generator code will calculate the increase in the quantity of water in the WP, the amount of each element dissolved in this water, the amount of each element lost due to the removal of water from the WP, the pH of the water, the solubility of materials in the water inside the WP, and the precipitation or dissolution of the species being tracked based on solubility. Uncertainties in parameters that will be used in these equations will be represented using the Monte Carlo technique. These uncertain parameters will be assigned distributions of possible values. Many realizations will be conducted by sampling a single value from the distributions of values assigned to all the uncertain parameters and calculating the results for each realization. The use of the Monte Carlo technique is fully described and evaluated in section 3.6 of this SER.

The NRC staff reviewed the methodology that the DOE will use to identify critical configurations against the acceptance criteria in the IRSRs to ensure that the proposed methodology, including the degradation models, geochemistry codes, differential equations used to track locations of materials, and the coefficients that will be used with these differential equations, will identify the configurations that have potential for nuclear criticality (CLST AC #5). The methodology uses models to develop the configurations of interest, but the acceptance of these computer codes is beyond the scope of the review of the TR.

The NRC staff found the use of corrosion models based on DOE material testing program and used in the TSPA for YM is acceptable to determine breach times of the WP and degradation rates of the WF and other components inside the WP. NRC staff found the use of a steady-state geochemistry code with modifications to track the quantity of water in the WP is acceptable to calculate the loss of fissionable elements and neutron absorbers and the composition of degradation products precipitating in the WP as long as the code is properly validated and verified. Additionally, NRC staff found the use of differential equations is acceptable to track the concentration of fissionable and neutron absorbing materials, as long as the coefficients for these equations are developed based on sufficient and appropriate data. NRC staff found the abstraction of the results from a steady-state geochemistry code is acceptable to develop the coefficients for these equations. Findings on the use of Monte Carlo calculations to simulate the uncertainty in the rates and locations of natural processes are found in section 3.6 of this SER.

**3.4.1.3 Internal Configuration Validation Approach**

The DOE proposes to not validate models that have been validated and used in the TSPA because the model validation will be evaluated during the LA review process for the repository. The degradation rates of internal components not modeled and validated in the TSPA will be developed from material test data and will be validated based on information and data provided as part of the disposal criticality analysis supporting the LA.

The geochemical code modified to track water movement of and used to determine the chemical environment inside the WP will be compared against analytical solutions and against results obtained by chaining several thousand individual EQ6 runs with adjustment of the water mass between runs. Additionally, the geochemical code will be validated by comparison to the other geochemistry-transport codes. The validation of specific computer codes is beyond the scope of this review, so no finding will be made as to the acceptability of the use of the EQ3/6 code for the repository environment.

The NRC staff reviewed the proposed methodology that the DOE will use to validate and verify the computer codes used to identify critical configurations against the acceptance criteria in the IRSRs. The methodology was reviewed to ensure that the approach to model validation and verification for the degradation models and geochemical codes will provide confidence that the codes will provide a reasonable representation of the configuration classes and configurations that may occur in the repository with a potential for nuclear criticality (TSPA AC #16 and AC #18). The acceptance of these computer codes is beyond the scope of the review of the TR. Modeling verification and validation of these computer codes will be evaluated when DOE submits the appropriate validation reports.

The NRC staff found the proposal to not validate models that have been validated and used in the TSPA is acceptable as long as the model is being used for the same purpose as it was used in the TSPA and no assumptions were made in the TSPA modeling that were conservative for purposes of performance assessment, but could be nonconservative for criticality analyses. The NRC staff will review the corrosion data supplied by the DOE and used as input in the model calculations during the review of DOE TSPA. The proposed methodology of validating and verifying the geochemistry code used to determine the chemical environment inside the WP by comparing the results of the code to analytical solutions, results obtained by chaining several thousand individual code runs, and results obtained using other geochemistry-transport computer codes is acceptable to the NRC staff. The acceptability of the EQ3/6 to model conditions expected in the repository has not been evaluated in this review, however. Additionally, NRC staff found that the proposed methodology for validation of the configuration generator code by comparing the results of the code to appropriate hand calculations is acceptable. In the LA, the DOE will have to provide verification that all computer codes used in the analysis are being implemented correctly and demonstrate that using these computer codes does not underestimate the probability of a criticality event for all WFs that will be disposed in the repository.

**3.4.2 External Configurations (Sections 3.1.2, 3.3, 4.2.3, 4.2.4.1, 4.2.4.2, 4.3.2, 4.3.3)**

The determination of external configurations is based on the parameter ranges of the variables that describe the potentially critical external configurations. In its responses to the RAI, DOE sought approval of the methodology for determining external configurations as part of the following request:

*DOE requests acceptance of the method for generating a comprehensive set of potential postclosure configurations as discussed in Sections 3.2 and 3.3 of the Topical Report.*

Two of the three principal components listed with this request are pertinent to external configurations:

- *Configuration generator: (1) Use of time-dependent first-order differential equations, solved by numerical integration, to track the concentration, or amount of fissionable or neutron absorber material; (2) Development of coefficients or terms of*

*these equations by abstraction from steady-state geochemistry code calculations; and (3) Random variation of terms or coefficients in these equations as part of a Monte Carlo calculation to reflect the uncertainty in the rates and location of natural processes.*

- *Accumulation Methodology: Ability of the methodology to calculate the accumulation of fissionable elements external to the waste package. For this purpose we are requesting acceptance of the use of a geochemistry-transport code and/or a geochemistry code used in a mode that simulates transport.*

In addition, the DOE in the RAI response requested acceptance for the approach to validating the configuration models in the following excerpts:

- *DOE also requests acceptance for the validation process for accumulation methodology that uses a geochemistry-transport code (e.g., PHREEQC, described in the response to RAI 4-32) or a geochemistry code used in a mode that simulates transport (e.g., EQ3/6 in the open-system mode described in Section 4.2.3).*
- *We also request acceptance that the configuration generator models described in Sections 4.3.3 and 4.3.4 can be validated by appropriate hand calculations.*

As discussed in section 3.3.2, the external criticality scenarios are grouped into configuration classes that define the particular sequence of FEPs that lead to a potentially critical configuration outside the WP. Within a configuration class, individual configurations reflect specific choices of parameters that define the input to criticality models. Staff assessment of the DOE external configuration methodology is addressed in three subsections, concerned with methodology, modeling, and validation approach.

**3.4.2.1 External Configuration Methodology**

In section 3.3 of the TR, the DOE briefly describes how it will develop these external configurations by quantifying parameter ranges for the configuration classes. Formulation of a configuration is based on parameters consistent with repository features, taking into consideration current design and site characterization. Examples listed include drift floor materials and host rock fracture density. The six steps for formulating a configuration are determinations of

- An FM source term using information from generation of internal configurations (section 3.4.1 of this SER)
- Water flow rates and patterns
- Sorption along flow paths
- Mineral precipitates along flow paths
- Alternate paths when primary rock fractures are filled, including possible coalescence of contaminant plumes from several WP
- Reaction products resulting from the plume encountering a reducing zone.

The technical basis for the overall approach to identifying configurations is not addressed explicitly, but it is tied to modeling and validation discussed elsewhere in the TR and reviewed in sections 3.4.2.2 and 3.4.2.3 of this SER.

Staff assessed the DOE method for generating external configurations with reference to NRC and DOE documents concerned with mechanisms of radionuclide release and transport in the repository environment. In particular, NRC IRSRs on the ENFE (Nuclear Regulatory Commission, 1999a) and RT (Nuclear Regulatory Commission, 1999b) KTIs provided extensive discussions on the range of FEPs that may affect the fate and transport of contaminants, including FMs and neutron absorbers in the NF and FF. AC from these IRSRs relevant to configuration methodology are section 2.3.3 items 3, 4, 14, and 16 (ENFE) and section 2.3.4 items 1, 2, and 8 (RT). Some of these criteria refer to specific choices of parameters and models—which are beyond the scope of this review—but the methodology was reviewed for the likelihood that it will address these criteria. There are other AC (e.g., concerned with mathematical modeling) that will need to be addressed by the DOE criticality analysis when it is performed for the LA. Also useful to this review were numerous discussions on these topics in the DOE technical basis report for the TSPA-VA (U.S. Department of Energy, 1998).

The NRC staff found that the proposed methodology for generating external configurations is sufficient to provide reasonable assurance that the analysis has been performed on a comprehensive set of external configurations and that no configuration that could substantially increase the calculated probability or consequence of a criticality event has been excluded. The method is appropriately tied to site and design features and involves a set of geochemical processes that encompasses realistic mechanisms for FM and neutron absorber fate and transport.

### 3.4.2.2 External Configuration Modeling Approach

For the portion of the analysis concerned with generation of external configurations, DOE requested acceptance of the use of a geochemistry-transport code, a geochemistry code used in a mode that simulates transport, or both to calculate FM accumulation external to the WP (SER section 3.4.2). Acceptance of specific codes was not requested. Section 3.4.2.1 of this SER discusses the DOE approach to constructing parameter ranges for potentially critical external configurations. The physical modeling—chiefly geochemical and hydrologic—applied in this effort is discussed separately in the TR. (Note that the present discussion does not include criticality modeling.)

As discussed in TR section 3.3, the DOE will take a systematic approach to determining the parameters essential to modeling the distribution of FM, neutron absorbers, and other physical and chemical features of external configurations that affect the criticality potential. External modeling will use geochemical models that include relevant geochemical processes and incorporate transport. At the time Revision 0 of the TR was prepared, central to this modeling was an “open system” geochemical transport model that was a manipulation of the zero-dimensional reaction code EQ3/6 (Wolery, 1992) to simulate one-dimensional water chemistry evolution, water-rock interaction, and FM deposition (section 4.2.3 and figure 4-7 of the TR). In the response to NRC RAI 4-32, the DOE stated that this model is expected to be replaced by the geochemical transport code PHREEQC (Parkhurst, 1995), supplemented by a modification of EQ3/6.<sup>2</sup>

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<sup>2</sup>Brocoum, S. *U.S. Department of Energy (DOE) Response to U.S. Nuclear Regulatory Commission (NRC) Request for Additional Information on the DOE Topical Report on Disposal Criticality Analysis Methodology*. Letter (November 19) to C.W. Reamer, Nuclear Regulatory Commission. Las Vegas, NV: U.S. Department of Energy. 1999.

Another component of external configuration modeling will be the configuration generator code (section 3.4.1.2). As for internal configurations, this code will provide bookkeeping for the transport between sites of application of a detailed geochemistry code and, in some situations, provide more rapid calculation where the detailed geochemistry code results can be used to develop heuristic models for the most significant ions for a few solution parameters. Section 4.3.3 of the TR describes how the code will be applied for geochemical tracking along pathways to two external settings, or "pond locations": the invert and the first "pond" external to the drift. For the invert, at each time step, the configuration generator code will accept the inflow from the WP and drift and then calculate the outflow decrement, pH and solubilities, precipitation/dissolution of appropriate solids, and, finally, concentrations in the outflow solution. For the initial path through the rock below the drift, the code will accept the outflow from the invert and then calculate the fracture travel time, matrix travel time, and outflow. The balance between use of the configuration generator code and the geochemistry models discussed in the previous paragraph has not been determined yet.

The DOE provided additional, clarifying information in its responses<sup>3</sup> to NRC RAI items 3-5, 3-9, 4-29, 4-31, 4-32, 4-37, 4-39, and 4-40 that resolved NRC questions on the external geochemical modeling approach. As noted earlier in this section, the response to RAI 4-32 (among others) states the DOE has changed what specific models it will use. The other RAIs concerned apparent deficiencies in the modeling approach suggesting that the models may not treat comprehensively all factors that can affect contaminant fate and transport. In each case, the DOE stated the relevant processes or mechanisms were, in fact, to be included in modeling as follows:

- RAI 3-5. Adsorption (which is one reason for the expected shift to PHREEQC)
- RAI 3-9. Temperature variation
- RAI 4-29. Kinetics
- RAI 4-31. Colloidal transport
- RAI 4-37 and 4-39. The range of water geochemical parameters in addition to pH
- RAI 4-40. Matrix-fracture distribution of flow

In each case, the DOE committed to providing language in a future TR revision to clarify that stated processes are merely examples. In many cases, the DOE provided more detailed, illustrative, technical discussions of expected modeling techniques, which made clear that their modeling approach was careful and comprehensive.

Staff assessed the DOE modeling approach for generating external configurations using the same documents and acceptance criteria listed as the basis for assessment of the methodology in section 3.4.2.1.

The NRC staff accept DOE use of a geochemistry-transport code, a geochemistry code used in a mode that simulates transport or both to calculate FM accumulation external to the WP. Such codes, when properly validated and applied, can provide reasonable estimates of contaminant (e.g., FM and neutron absorbers) disposition. These codes can also allow calculation of bounding cases that can support an argument of reasonable assurance that no configuration that could substantially increase the calculated probability or consequence of a criticality event has been excluded. Properly applied geochemical codes

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<sup>3</sup>Brocoum, S. *U.S. Department of Energy (DOE) Response to U.S. Nuclear Regulatory Commission (NRC) Request for Additional Information on the DOE Topical Report on Disposal Criticality Analysis Methodology*. Letter (November 19) to C.W. Reamer, Nuclear Regulatory Commission. Las Vegas, NV: U.S. Department of Energy. 1999.

(in conjunction with natural analog data) provide a bridge between laboratory or field test data and long-term prediction and have been applied extensively in other components of the repository program (e.g., U.S. Department of Energy, 1998). This approval is contingent on a satisfactory revision of the TR that addresses the RAIs discussed in this section.

### 3.4.2.3 External Configuration Validation Approach

The DOE has requested acceptance of the validation approach for the external accumulation modeling methodology and the configuration generator code. In enclosure 2 of the RAI response,<sup>4</sup> the DOE stated that accumulation modeling validation will include “comparison between codes (both EQ3/6 and PHREEQC), comparison with experimental data, and comparison with natural analogs.” Acceptance was not requested for bounding cases, nor for the results of any validation exercises. In addition, configuration generator code validation was described as involving hand calculations to check species tracking.

Because the DOE is not requesting acceptance of specific codes, this review will view the validation process generically. One component of the process is comparison among different codes; the examples presented by DOE<sup>5</sup> being between PHREEQC and either the linked EQ6 runs (section 4.2.3 of the TR) or a modification of EQ6 that incorporates a Lagrangian transport model (response to RAI 4-33). Code comparison does not provide direct evaluation against actual data, but may provide an extra measure of confidence beyond validation. The second component of validation mentioned in the response to RAI 4-33 is comparison “against more complex analytical solutions for reactive transport.”<sup>6</sup> This process is not described further, and so cannot be evaluated. The third validation component is “against experimental data (both laboratory and natural analogs).”<sup>7</sup> The RAI 4-33 response lists some examples of such validation for reactive transport codes with reference to the applicability of parameters such as Peclet and Damköhler numbers, flow rates, and water chemistry. Similarly, the response discusses criteria for selecting appropriate laboratory data for validation purposes, and cites ongoing studies that may prove useful for benchmarking. The DOE committed to discuss codes not covered in the TR (PHREEQC and Lagrangian modified EQ3/6) in the revised TR.

Laboratory and natural analog data validation cases for EQ3/6 are depicted in tables 4-2 and 4-3 of the TR; because specific codes are not under consideration for acceptance in this SER, these tables were reviewed only as examples. NRC RAI 4-33 raised topics of applicability and bounding with regard to these validation cases; the conditions under which EQ3/6 has been validated, as reported in the TR, are not analogous to either the modeled in-drift conditions that may include WP corrosion products nor to the external conditions of low-temperature interaction between drift effluent and tuff fractures. The DOE responses discussed in the preceding paragraph were targeted to those critiques. DOE acknowledged in TR section 4.2.4.2 that reaction rates are highly uncertain and not constrained by the validation exercises.

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<sup>4</sup>Brocoum, S. *U.S. Department of Energy (DOE) Response to U.S. Nuclear Regulatory Commission (NRC) Request for Additional Information on the DOE Topical Report on Disposal Criticality Analysis Methodology*. Letter (November 19) to C.W. Reamer, Nuclear Regulatory Commission. Las Vegas, NV: U.S. Department of Energy. 1999.

<sup>5</sup>Ibid.

<sup>6</sup>Ibid.

<sup>7</sup>Ibid.

Beyond validation, another means for increasing confidence that the modeling of external accumulations has not resulted in the exclusion of configurations that would increase the probability or consequence of criticality is sensitivity studies. For example, a poorly constrained geochemical parameter, such as a solubility product that controls the quantity of an FM in a certain configuration class, may be varied from one run to another to ensure that model results do not change significantly in response to changes in the parameter value. In its response to RAI 4-34, the DOE described an example sensitivity analysis that, while directed to in-package chemistry, also serves to illustrate external cases. The DOE, however, does not explicitly state that it will perform such analyses for the criticality analysis supporting the LA.

For validation of the configuration generator code, the DOE proposes to use hand calculations. This approach is based on the fact that the configuration generator code is a bookkeeping tool that does not simulate physical or chemical processes—it merely serves to track the results of such simulations.

Staff assessed the external configuration model validation approach with reference to the following IRSR acceptance criteria listed in this SER: ENFE items 12 and 13 (section 2.3.3) and RT item 4 (section 2.3.4).

Staff approve the DOE validation process for external accumulation modeling as exemplified by tables 4-2 and 4-3 of the TR and as summarized in the response to RAI-33.<sup>8</sup> This acceptance is contingent on

- TR revisions regarding code descriptions promised in that response
- More detailed description in the revised TR of the geochemical code validation process, perhaps modeled on the discussion in the RAI 4-33 response and including additional details on the comparison against more complex analytical solutions for reactive transport
- The DOE's use in the criticality analysis of the principles of selection of appropriate and bounding laboratory and natural analog data as discussed in that response, in recognition of the insufficiency of the lists in tables 4-2 and 4-3 of the TR
- The DOE's use in the criticality analysis of uncertainty and sensitivity analyses provides reasonable assurance that, as a result of uncertainties in parameter values, modeling has not excluded configurations that would increase the probability or consequence of criticality.

Additionally, the proposed methodology for validation of the configuration generator code by comparing the results of the code to appropriate hand calculations is acceptable. In the LA, the DOE will have to provide verification that these computer codes are being implemented correctly and demonstrate that the use of these computer codes does not underestimate the probability of a criticality event for all WFs disposed in the repository.

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<sup>8</sup>Brocoum, S. *U.S. Department of Energy (DOE) Response to U.S. Nuclear Regulatory Commission (NRC) Request for Additional Information on the DOE Topical Report on Disposal Criticality Analysis Methodology*. Letter (November 19) to C.W. Reamer, Nuclear Regulatory Commission. Las Vegas, NV: U.S. Department of Energy. 1999.

### 3.6 Probability of Critical Configurations (Sections 3.5, 4.3, 4.3.1, 4.3.2, 4.3.3, 4.3.4)

In its responses to the RAI, DOE has requested an approval of the methodology for determining the probability of critical configurations as stated by the DOE in the following:

*DOE requests acceptance of the following aspects of the probability estimation method: (1) Development and use of a table of  $k_{eff}$  for the range of possible configuration parameters to construct a regression for  $k_{eff}$  as a function of these parameters or for direct table lookup and interpolation (Section 3.5, page 3-21 and modification of this paragraph given in the response to RAI 3-16); (2) Monte Carlo methodology using random sampling of parameters characterizing configurations and determination of  $k_{eff}$  by calculation from the regression expression or table lookup and interpolation as a function of these parameters to obtain a sample of up to 1 million values of  $k_{eff}$  to simulate a probability distribution (the new paragraph for the Topical Report, given in the response to RAI 3-16); (3) Incorporation of the WAPDEG-generated probability distribution for time of breach and duration of the "bathtub" as two of the parameters (Section 3.5, page 3-22); and (4) Estimate of criticality risk for TSPA (before 10,000 years and to the time of peak dose) (paragraph to be included at the end of Section 3.7, attached to the response to RAI C-14). Acceptance of this item is requested in Section 1.2, Part E of the Topical Report.*

*DOE requests acceptance of the validation process for the probability calculation and configuration generator models presented in Sections 3.5 and 4.3 of the Topical Report as modified by responses to RAIs 3-16, 3-19, 4-25, 4-36, and 4-37 that will be implemented by the Monte Carlo probability calculation methodology. DOE plans to validate this methodology by comparison with hand calculations of combinations of probabilities of individual events taken from distributions similar to those used for the Monte Carlo selection process. We also request acceptance that the configuration generator models described in Sections 4.3.3 and 4.3.4 can be validated by appropriate hand calculations.*

#### 3.6.1 Probability Methodology

The probability of a critical configuration is determined by first identifying the configuration classes that have a  $k_{eff}$  exceeding the critical limit over a portion of their parameter range. This screening uses a multivariate regression for  $k_{eff}$  as a function of WF burnup, enrichment, and cooling times. These regressions will be developed using a commercial neutron transport code such as MCNP (Oak Ridge National Laboratory, 1997) for representative values of these parameters and will be based on the upper 95<sup>th</sup> percent confidence level of the regression such that configuration classes are not likely to be improperly screened due to uncertainty in the regression. The development of the regression equation for  $k_{eff}$  is evaluated in section 3.5 of this SER.

The scenario and configuration parameters are assigned probability distributions based on their uncertainty, and the Monte Carlo technique is used to estimate criticality probability. The Monte Carlo technique consists of a random selection of parameter values from the parameter distributions and determination of whether the selected parameter values satisfies the requirements for criticality. This

process of selecting parameter values and determining whether the associated configuration yields a criticality event is repeated many times to yield an estimate of the probability of a critical configuration. Correlations among sampled parameters will be accounted for by using appropriate conditional probability distributions for sampling parameters that depend on previously sampled parameters, as indicated in the DOE response to RAI 4-35. The criticality analysis will use the WAPDEG-generated probability distributions for the time of WP breach and duration of the "bathtub" (i.e., the pooling of water within this WP) associated with the most recent TSPA.

The NRC staff reviewed the proposed methodology to determine the probability of occurrence of a criticality event against the acceptance criteria in the IRSRs. The methodology was revised to ensure that it will be sufficient to provide reasonable assurance that DOE has developed a technically defensible, transparent, and traceable method to assign probability values to criticality scenario classes, scenarios, configuration classes, and configurations (CLST AC #6) and has adequately addressed the uncertainty in data due to both temporal and spatial variations in conditions affecting potential nuclear criticality (TSPA AC #14).

The NRC staff found the proposed methodology of using the Monte Carlo technique to account for uncertainty in data to determine the probability of critical configurations is acceptable. The NRC staff found this technique will allow DOE to provide reasonable assurance that the probability of postclosure criticality at the repository will not be underestimated. Acceptance is contingent on DOE incorporating the steps stated in the response to RAI 3-16 if there is a problem using a regression to represent a parameter. The NRC staff found the use of the WAPDEG-generated probability distributions for the time of WP breach and duration of the "bathtub" inside the WP associated with the most recent TSPA is acceptable provided the DOE can demonstrate that no assumptions were made in the WAPDEG modeling that would be conservative for TSPA calculations, but nonconservative for criticality calculations. The acceptability of the methodology to generate the regression equation to determine  $k_{\text{eff}}$  has been evaluated in section 3.5 of this SER. The acceptability of the methodology to determine the risk from criticality has been evaluated in section 3.8 of this SER.

### 3.6.2 Probability Modeling Approach

Because the potential of a criticality event occurring changes through time as the rate of infiltration to the drift changes, WPs fail, and materials within the WP are redistributed, the neutron multiplication factor must be calculated for many time steps to ensure that the criticality potential of a realization has been evaluated properly. The DOE calculation of the probability of occurrence of an internal criticality will consist of the following steps, as illustrated in figure 4-8a of the DOE TR:

1. Sample from the distribution of infiltration to the drift from the most recent version of TSPA.
2. Sample from the distribution of failure times determined by the TSPA programs WAPDEG and RIP from the drip rate sampled in step 1. WAPDEG is the code that calculates the failure times and conditions for WP degradation and RIP is the executive driver for the DOE's TSPA program. Per response to RAI 4-25, these failure times will be based on corrosion rates determined by testing programs at Lawrence Livermore National Laboratory and the University of Virginia.
3. Sample the height of WP penetration to determine the water level in the package.

4. Sample the WF characteristics including enrichment, burnup, and cooling time and determine whether this fuel has the potential to yield a criticality event by comparing these characteristics to the bonding characteristics needed to achieve criticality (i.e., the critical limit derived previously). The realization is ended if the fuel cannot yield a criticality event inside the WP.
5. Sample the degradation rates of the WF and the internal components of the WP, accounting for correlations as appropriate.
6. Calculate the amounts of neutronically significant material remaining in the WP using the degradation state of the WF and the internal components as inputs to the configuration generator code or the detailed calculations of a geochemistry code such as EQ3/6 (Wolery, 1992).
7. Test whether the  $k_{\text{eff}}$  of the configuration analyzed exceeds the critical limit. The realization is ended if  $k_{\text{eff}}$  exceeds the critical limit.
8. Check whether the ending condition has been reached and if not, increment the time and return to step 6. The ending condition is typically a time limit or the time at which a hole develops in the bottom of the WP, water is released, and criticality within the WP is no longer possible.

The probability of criticality will be calculated as the number of realizations that produced a critical configuration of FM divided by the total number of realizations. This process will be repeated for a sufficient number of realizations to yield a sufficiently small uncertainty in the probability of criticality. Per response to RAI 3-16, the DOE has indicated that preliminary estimates of the number of realizations required to drive the uncertainty to an acceptably small number is about  $10^8$ .

Similar to the calculation of the probability of an internal criticality, the calculation of the probability of occurrence of an external criticality will be conducted with a Monte Carlo calculation and will consist of the following steps, as illustrated in Figure 4-8b of the DOE TR:

1. Sample the flow rate, concentration of FMs, and pH of the water flowing out of the WP.
2. Sample the external path leading to an external criticality location, the transport parameters, and the accumulation parameters. Parameters sampled to determine the location of accumulation include the groundwater flow rate, rock porosity, and the fracture density. Parameters sampled to determine the transport and accumulation properties of materials will include adsorption coefficients and will be consistent with the TSPA.
3. Calculate the amounts of fissionable material removed from the flow in the external environment. Geochemical analyses will be utilized to identify the portions of the external environment that can remove fissionable material from the flow and determine the chemical environment in these locations.
4. Evaluate the  $k_{\text{eff}}$  of configurations having a significant accumulation of FM. If the  $k_{\text{eff}}$  of the maximum concentration of FM exceeds the critical limit, it is recorded and a new realization is started.

The probability of criticality will be calculated as the number of realizations that produced a critical configuration of FM divided by the total number of realizations. This process will be repeated for a sufficient number of realizations to yield a sufficiently small uncertainty in the probability of criticality. The ranges and distributions of most of the parameters sampled will be provided by the inputs into and results of the most recent TSPA.

The NRC staff reviewed the proposed modeling approach to determine the probability of occurrence of a criticality event against the acceptance criteria in the IRSRs. The modeling approach was reviewed to ensure that DOE has developed a technically defensible, transparent, and traceable method to assign probability values to criticality scenario classes, scenarios, configuration classes, and configurations (CLST AC #6) and has adequately addressed the uncertainty in data due to both temporal and spatial variations in conditions affecting potential nuclear criticality (TSPA AC #14).

The NRC staff found the use of the Monte Carlo technique is an acceptable method to determine the probability of critical conditions occurring based on configurations defined by multiple uncertain parameters. The NRC staff consider the use of data from the most recent TSPA in the criticality evaluation an acceptable source of the input data for the probability calculation by NRC staff as long as correlations among parameters are accounted for in the sampling scheme and the ranges from the TSPA are not conservative estimates for the calculation of dose but nonconservative for criticality calculations. For example, the TSPA may use an unrealistically low value for the  $K_d$  of plutonium in the unsaturated zone to be conservative. This value for the  $K_d$  of plutonium may not be appropriate in the criticality calculations because a higher  $K_d$  could lead to a greater amount of accumulation of plutonium and a higher potential for criticality.

### 3.6.3 Probability Validation Approach

DOE proposes to validate the code that incorporates this Monte Carlo methodology using hand calculations and a commercial mathematical equation solver code to verify that the Monte Carlo code is properly sampling from the input parameter distributions and calculating the probability correctly. One example of the type of hand calculation that could be used in this validation process is fixing the value of sampled parameters to ensure that the code reproduces results that can be verified using an equation solver code.

The NRC staff reviewed the proposed approach to validate the models that will be used to determine the probability of occurrence of a criticality event against the acceptance criteria in the IRSRs. The validation approach was reviewed to ensure that DOE has developed a technically defensible, transparent, and traceable method to assigning probability values to criticality scenario classes, scenarios, configuration classes, and configurations (CLST AC #6).

The NRC staff found the methodology of using hand calculations and a commercial mathematical equation solver code to verify that the Monte Carlo code is properly sampling from the input parameter distributions and calculating the probability correctly is considered acceptable by NRC staff provided that a sufficient number of these calculations are conducted to demonstrate that the code is performing the calculations properly across the range of the sampled parameters. In the LA, DOE will have to provide verification that these computer codes are being implemented correctly and demonstrate that the use of these computer codes does not underestimate the probability of a criticality event for all WFs that will be disposed in the repository.

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